Roton Induced Modulations in Underdoped Cuprates as a Signature of Incipient Electronic Order

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In the last years there have been measurements of energy independent modulations in underdoped cuprates via scanning tunnelling microscopy. These modulations of around 4 lattice constants occur near vortex cores in samples with and without superconductivity, and in the pseudogap regime of some superconducting samples. Recently, it was proposed that the origin of the modulations is electronic charge ordered phases intrinsic to doped Mott insulators. We show that even if the system has not charge ordered, proximity to such an order will induce modulations at the same ordering wavevector. Such modulations are a signature of the real or incipient order. We construct ground state wavefunctions that include strong fluctuations of the competing order without having ordered. They exhibit deep roton minima at wavevectors of the reciprocal lattice of the incipient order due to proximity to the phase transition into the charge ordered state. Such minima, in turn, produce strong modulations. Moreover, the effects are generic and are present whenever an electronic system is near a crystalline phase. This leads to experimental signatures even if the electronic system has not solidified. The signatures will be ubiquitous near the dopings that stabilize the electronic order.

In the present note we would like to point out that the recent proposed explanation[1] for STM modulations at certain doping dependent wavevectors in samples with and without superconductivity, and around vortex cores[2] is of a quite general nature. The modulations around the vortex core were predicted in the context of the $SO(5)$ picture of high T_c[3], but their nature is more general than the specific model. We show more directly how the physics comes about by means of a quantum mechanical density functional formalism. The proposal[1] is of an enhanced charge susceptibility due to charge order or to a deep roton minimum at certain wavevectors. We show that roton induced modulations are always present near a solidification quantum transition regardless of whether the electron system has charge ordered or not. Therefore the experimental signatures should be quite generic and rather common as long as one is close to an electronic crystal phase.

That roton physics follows on quite general grounds can be inferred from the experimental properties of bosonic systems. Helium is a superfluid at zero temperature, but it is an almost solid barely melted by quantum fluctuations. An indication of its proximity to the solid phase is the deep roton minimum in the excitation spectrum[4, 5] or, equivalently, the peak in the structure factor at the same wavevector. On the other hand, artificially engineered superfluids such as atomic BECs[6], which are not near a solid transition by experimental design, do not have a peak in the structure factor[7] and hence they will not have a roton excitation unless they are tuned near a Mott transition.

In the case of the cuprates there is a plethora of possible Coulombic stabilized insulating phases: the low doping antiferromagnetic insulator, stripes[8], hole Wigner crystals[1] and even a semimetallic orbital

antiferromagnet[9], among others. Whenever one of these phases *with charge order* (stripes, Wigner crystals, charge density waves) becomes competitive in energy with the superconductivity, an incipient Bragg peak will start forming, producing enhanced fluctuations at appropriate wavevectors and thus a spike in the structure factor. This spike leads to a roton minimum in the excitation spectrum [5, 10]. In fact, the magnetic neutron (π, π) mode[11] is such a roton minimum in the spin rather than charge density excitation spectrum. It is due to proximity to an electron crystal phase, the antiferromagnetic insulator, at very low dopings[9].

The Hamiltonian

$$\mathcal{H} = \int \left(m \frac{\vec{v} \cdot \rho \vec{v}}{2} \right) d^3r + U[\rho] \tag{1}$$

describes quantum many particle systems [4]. $\vec{v} \cdot \rho \vec{v}/2$ is the kinetic energy operator, $U[\rho]$ is the potential energy operator, which in general can be a functional of the density operator. The density operator in first quantized notation is

$$\rho(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i) \tag{2}$$

with $\vec{r}_i$ being the position of the ith particle. The velocity operator is in first quantized notation

$$\vec{v}(\vec{r}) = \sum_i \left[\frac{\vec{p}}{2m} \delta(\vec{r} - \vec{r}_i) + \delta(\vec{r} - \vec{r}_i) \frac{\vec{p}}{2m} \right] \tag{3}$$

with commutation relation

$$[\rho(\vec{r}\,'), \vec{v}(\vec{r})] = i\frac{\hbar}{m} \nabla \delta(\vec{r}\,' - \vec{r}) \tag{4}$$

The ground state of the Hamiltonian (1) could be a quantum liquid or solid depending on the interaction. Since

our main concern is how a crystallization transition is approached, we will suppose it to be a liquid, of course a superconductor for the case of the cuprates, but our considerations are more general.

We study the nature of the density excitation spectrum of the fluid on quite general grounds by the methods of Landau and the Russian school[12]. We suppose the density to have a well defined average which we take to be uniform for simplicity. This will not change the nature of the considerations, although in real life the density can be modulated by the lattice. The average velocity is zero as we consider a system at rest. We Fourier expand the density and velocity operators about their averages:

$$\rho(\vec{r}) = \rho_0 + \frac{1}{N}\sum_{\vec{k}}\rho_{\vec{k}}e^{i\vec{k}\cdot\vec{r}} \tag{5}$$

$$\vec{v}(\vec{r}) = \frac{1}{N}\sum_{\vec{k}}\vec{v}_{\vec{k}}e^{i\vec{k}\cdot\vec{r}} \tag{6}$$

where we are using the lattice normalization, the number of sites N instead of the volume V. Quantum mechanically, the velocity is proportional to the gradient of the local phase variable of the particle, $\vec{v}(\vec{r}) = \hbar/m\nabla\theta$, or in Fourier components

$$\vec{v}_{\vec{k}} = \frac{i\hbar\vec{k}}{m}\theta_{\vec{k}} \tag{7}$$

The density velocity commutation relation (4) implies the well known density phase commutation relation

$$[\,\rho_{\vec{k}}\,,\,\theta_{-\vec{k}'}\,] = i\delta_{\vec{k}\vec{k}'} \tag{8}$$

i.e. $\hbar\theta_{-\vec{k}}$ is the momentum conjugate to the density fluctuation $\rho_{\vec{k}}$. The Hamiltonian (1) thus becomes

$$\mathcal{H} = U(\rho_0) + \frac{1}{N}\sum_{\vec{k}}\left\{\frac{\rho_0\hbar^2k^2}{2m}|\theta_{-\vec{k}}|^2 + \frac{1}{2}\left(U_{\vec{k}} + \frac{\hbar^2k^2}{4m\rho_0}\right)|\rho_{\vec{k}}|^2\right\} \tag{9}$$

where $U_{\vec{k}}$ is the Fourier transform of the interaction and $(\hbar^2k^2)/(4m\rho_0)|\rho_{\vec{k}}|^2$ is the elastic energy associated with changing the density. This last term comes from acting the Hamiltonian on the wavefunction and making sure that one keeps careful track of both density and phase degrees of freedom[13] in the full quantum mechanical kinetic energy term.

We see that the quantum liquid is a collection of harmonic oscillators in momentum space for the density fluctuations. The mass of the oscillators is given by

$$M_{\vec{k}} \equiv \frac{m}{\rho_0k^2} \tag{10}$$

and spring constant by

$$K_{\vec{k}} \equiv U_{\vec{k}} + \frac{\hbar^2k^2}{4m\rho_0}\,. \tag{11}$$

The density energy excitation spectrum of the quantum liquid is

$$E_{\vec{k}} = \hbar\omega_{\vec{k}}(n + 1/2) \tag{12}$$

$$\omega_{\vec{k}}^2 = \frac{K_{\vec{k}}}{M_{\vec{k}}} = \frac{\rho_0k^2}{m}\left(U_{\vec{k}} + \frac{\hbar^2k^2}{4m\rho_0}\right) \tag{13}$$

The ground state energy is given by $U(\rho_0) + \sum_{\vec{k}}\hbar\omega_{\vec{k}}/2$. We note that the Virial theorem implies that

$$\frac{1}{2}\hbar\omega_{\vec{k}}N = \left(U_{\vec{k}} + \frac{\hbar^2k^2}{4m\rho_0}\right)\langle|\rho_{\vec{k}}|^2\rangle$$

$$\hbar\omega_{\vec{k}} = \frac{\hbar^2k^2}{2mS(\vec{k})} \tag{14}$$

where the structure factor is defined by

$$S(\vec{k}) = \frac{\langle|\rho_{\vec{k}}|^2\rangle}{N\rho_0} \tag{15}$$

which is, of course, the Fourier transform of the density-density correlation function. For the quantum liquid we thus have

$$S(\vec{k}) = \frac{\hbar k}{2m}\frac{1}{\sqrt{\frac{\rho_0}{m}\left(U_{\vec{k}} + \frac{\hbar^2k^2}{4m\rho_0}\right)}} \tag{16}$$

The ground state energy will have the density oscillators unexcited. Hence, if the ground state wavefunction of the electronic system *without density correlations* is $|\psi_{GS}\rangle$, the ground state wavefunction *with density correlations* is

$$|\psi\rangle = \exp\left\{-\frac{1}{2}\sum_{\vec{k}}\sqrt{\frac{m}{\rho_0\hbar^2k^2}\left(U_{\vec{k}} + \frac{\hbar^2k^2}{4m\rho_0}\right)}|\rho_{\vec{k}}|^2\right\}|\psi_{GS}\rangle\,. \tag{17}$$

The factor in front appears because it is the ground state wavefunction of harmonic oscillators. The ground state wavefunction has the oscillators shaking as little as possible. We see that the factor suppresses density fluctuations. The wavefunction is essentially exact to quadratic order in the density fluctuations. This way of including correlations was pioneered by Bohm and Pines[14] and is known colloquially as the RPA. This correlated ground state wavefunction is a Jastrow type wavefunction analogous to the Laughlin Fractional Quantum Hall wavefunction[13].

One could play the same game as for the ground state wavefunction (17) and write down the excited state wavefunctions for the density oscillators. On the other hand, these collective density oscillations are mostly not good approximations to eigenstates of the system since they

will readily decay into particle-hole pairs except at the longest wavelengths. Such long wavelength oscillations are plasmons, for which the present consideration leads readily to $\omega_{\vec{k}}^2 = 4\pi e^2 \rho_0/m$, as for the electron Coulomb interactions we have $U_{\vec{k}} = 4\pi e^2/k^2$ which dominate as $\vec{k} \to 0$.

The ground state wavefunction (17) does not contain any electronic crystalline order as $\langle \rho_{\vec{k}} \rangle = 0$ for all $\vec{k}$. When the electron system solidifies, either spontaneously or lattice induced, it will exhibit Bragg peaks at the reciprocal lattice vectors corresponding to the electron crystal. These peaks mean that $\langle \rho_{\vec{Q}} \rangle \neq 0$. We are interested in the case when the electron system solidifies spontaneously, and in particular, in its behavior as it approaches such a point.
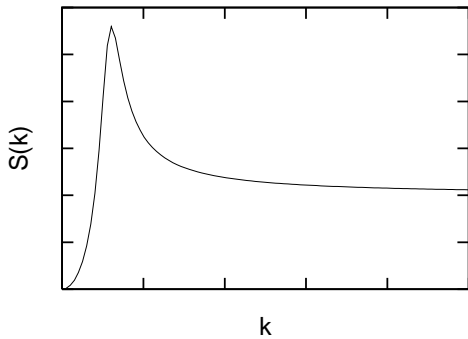

FIG. 1: Structure factor vs. momentum. The roton maximum is easily visible.

As the electron fluid approaches spontaneous crystallization with reciprocal wavevector $\vec{Q}$ for the incipient order, there will be enhanced density fluctuations $\langle |\rho_{\vec{Q}}^2| \rangle$ at such a wavevector. This follows because proximity to the crystallization softens the density oscillators of the electron liquid, $\vec{K}_{\vec{Q}} \to 0$, which makes $\omega_{\vec{Q}} \to 0$. Hence the interaction $U_{\vec{k}}$ has a minimum at $\vec{Q}$. The softening of the density mode thus produces a peak in the structure factor, $S(\vec{k})$, that diverges as one approaches the point when the system solidifies. This peak will drag the spectrum down according to the equation (14) creating a roton minimum[5, 10] that can be thought of as an exciton. We thus have as a simple phenomenological model that captures the physics

$$U_{\vec{k}} = \frac{4\pi e^2}{k^2} + \alpha \frac{\hbar^2}{4m\rho_0}(\vec{k} - \vec{Q})^2 - \frac{4\pi e^2}{Q^2}$$
$$+ \alpha \frac{\hbar^2 Q^2}{4m\rho_0} - \alpha \frac{\hbar^2 k^2}{4m\rho_0} + \Delta_{\text{roton}} \quad (18)$$

where nonzero α makes a roton minimum, and Δ_{roton} is the roton gap, which will collapse at the crystallization transition as the smallness of the gap of such a roton is a measure of proximity to crystallization. From the form

of the interaction we get the structure factor and the density excitation spectrum, which we plot in Figures 1 and 2, where the roton wavevector was chosen arbitrarily as 1, α was chosen as $1/2$, the roton gap Δ_{roton} as $1/4$ and all other dimensionful constants were chosen to have unit scale.

We consider the case when an external potential $-V_{\vec{k}}$ acts on the electrons thus adding a term

$$\mathcal{H}_{\text{ext}} = - \sum_{\vec{k}} V_{\vec{k}} \rho_{\vec{k}} . \quad (19)$$

The external potential might be the ionic lattice or it might be the impurity potential. The effect of the extra term in the ground state wavefunction is to move the equilibrium position of the density oscillators from $\langle \rho_{\vec{k}} \rangle = 0$ to

$$\langle \rho_{\vec{k}} \rangle = \frac{V_{\vec{k}}}{U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0}} . \quad (20)$$

We point out that when $V_{\vec{k}}$ is the lattice potential, this is just the electron fluid acquiring the periodicity of the underlying lattice with appropriate Bragg peaks.
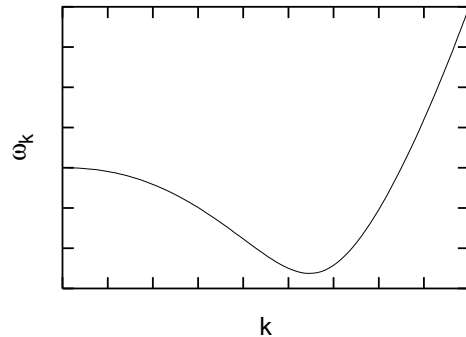

FIG. 2: Density oscillation frequency vs. momentum. The plasmon gap and the roton minimum are easily visible.

When the electron fluid is near a solidification transition with reciprocal lattice vector $\vec{Q}$ for the incipient order, there will be a large enhancement of the density component at or near wavevector $\vec{Q}$ due to the roton minimum unless $V_{\vec{k}} \equiv 0$ for the region around the minimum. In figure 3 we plot the enhancement of the density Fourier component for a constant potential which could correspond to a localized impurity. The scale of the potential in the figure was chosen arbitrarily as 1. On the other hand, we stress that the effect is general and the enhancement will be there for the lattice potential. Quasiparticles will scatter strongly of the roton enhanced density Fourier components at and around $\vec{Q}$. These corroborates the previous suggestions[1] and we thus identify this enhancement with the STM[2] bias independent signatures.

We point out that our result shows the generality of the roton induced modulations near an electronic crystal phase effect, and that charge order is not necessary for the observation of the experimental signatures. The physics follows because it is very easy to make density fluctuations at the roton wavevectors. Since the electron density is very high at roton wavevectors, there will be an enhanced charge susceptibility at such wavevectors leading to modulations[1] *as long* as the system is near enough to an electronic crystal phase. The phenomenon can be observed in superconducting samples which might not have the charge order. For example, in underdoped samples if superconductivity is lost at a temperature not far above the roton gap, these modulations will be present. Since T_c collapses with underdoping, the modulations will be easier to observe for small doping.
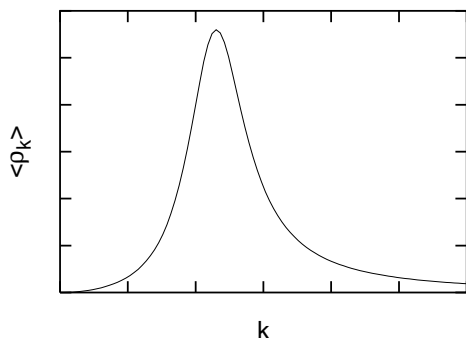

FIG. 3: Density Fourier component vs. wavevector. The enhancements of the density Fourier components at and around the roton wavevector are easily visible.

Measurements of metallic like conductivity below the Neel temperature[15] in underdoped cuprates, Hall effect[15] transport measurements, and the different photoemission properties of nodal vs. antinodal quasiparticles[16] have as the simplest explanation that there are two types of electronic carriers in underdoped cuprates. It is certainly suggestive that the experimental wavevectors for the modulations are in the antinodal directions[2]. The roton model will be a two fluid system as there will be low energy quasiparticles near the roton minimum which will behave more like excitations of the competing insulating order, while low energy quasiparticles coming from other wavevectors will tend to behave like superconducting Bogolyubov-BCS excitations.

We finally point out that there are reports of a Boomerang effect in the cuprates[17]. This consists in T_c becoming proportional to superfluid density, n_s, in the overdoped regime as a consequence of a decreasing number of superconducting electrons. This suggests a loss of spectral weight of the superconducting phase to a competing order. If the roton minima are indeed signatures of incipient electronic crystal phases and the competing phase on the overdoped side is an electronic crystal, there

will be similar modulations in the overdoped regime observable in STM experiments.

We would like to mention that recently there was also a proposal that the STM modulations are a Copper pair crystal[18]. On similar physical grounds as expressed in[1], we believe such a crystal would not occur, but we emphasize that the two proposals are differentiable experimentally according to at which doping one observes specific modulations. We also stress that the physics we have described is more general than either proposal because as long as there is an incipient solid order, there will be roton minima at its reciprocal wavevectors and the concomitant modulations.

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